Some remarks on the visible points of a lattice

M Baake†‡, U Grimm‡§ and D H Warrington‖

† Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Federal Republic of Germany
‡ Department of Mathematics, The University of Melbourne, Parkville, VIC 3052, Australia
§ Instituut voor Theoretische Fysica, Universiteit van Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands
‖ School of Materials, The University of Sheffield, Mappin Street, Sheffield S1 3JD, UK

Abstract. We comment on the set of visible points of a lattice and its Fourier transform, thus continuing and generalizing previous work by Schroeder and Mossen. A closed formula in terms of Dirichlet series is obtained for the Bragg part of the Fourier transform. We compare this calculation with the outcome of an optical Fourier transform of the visible points of the 2D square lattice.

Recently, Mosseri has given a nice and elegant description of the set of visible points of a lattice (i.e. those points except the origin that connect to the origin via a straight line without hitting any other lattice point in between) and some of its properties [2], continuing previous work by Schroeder [1, 3]. Both authors are most interested in the Fourier transform of this set. Unfortunately, the results of these two attempts are contradictory. The algebraic approach of [2] is essentially correct, but contains a couple of mistakes and unnecessary restrictions. In what follows, we add several remarks to straighten this out and then compare the 2D case with an optical experiment.

Let $\Lambda = \mathbb{Z}b_1 \oplus \cdots \oplus \mathbb{Z}b_n$ be a lattice in nD space with linearly independent basis vectors $b_1, \ldots, b_n$. The set F_Λ of visible points [2–4] can be characterized as

$$F_\Lambda = \{m_1 b_1 + \cdots + m_n b_n \mid \gcd(m_1, \ldots, m_n) = 1\} \tag{1}$$

where gcd denotes the greatest common divisor. This set does *not* include the origin with respect to which it is defined. We follow [2] for the notation as far as possible.

The set F_Λ is non-periodic and is left invariant by the group of lattice automorphisms, Aut(Λ), which is isomorphic to $Gl(n, \mathbb{Z})$, the group of integer $n \times n$ matrices with determinant ± 1. This is seen from $M \in$ Aut(Λ) transforming fundamental cells of the lattice to other fundamental cells and hence visible points to visible points [4, 6]. As a consequence, the set of visible points admits precisely the same point symmetry as the lattice Λ itself, the transformations are not restricted to pure rotations. This can clearly be seen from figure 1 which shows the case of the square lattice.

How frequent are visible points? If p denotes the probability of a lattice point to be visible (defined through a volume limit which exists, compare ch. 3.8 of [7]), we also have ($\ell \in \mathbb{N} = \{1, 2, 3, \ldots\}$) the probabilities

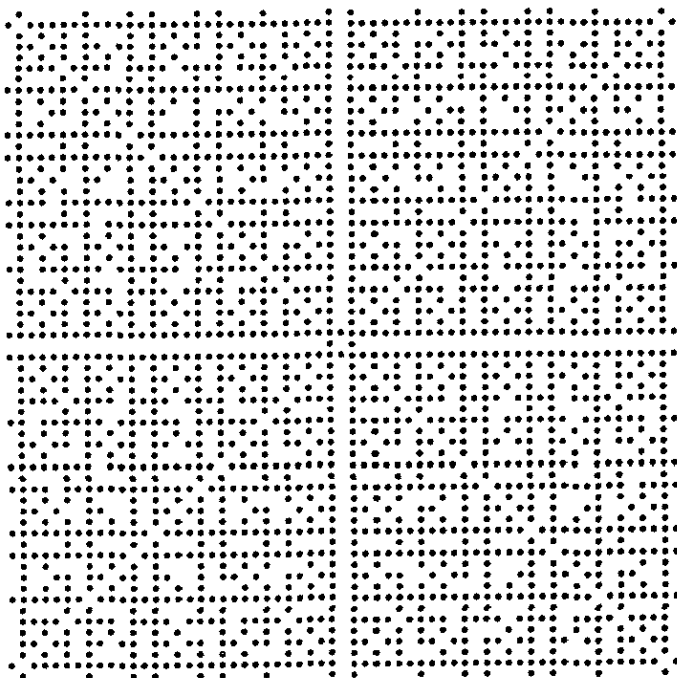$$P(x \in \ell \cdot F_\Lambda) = \frac{p}{\ell^n} \tag{2}$$

Figure 1. Some visible points of the 2D square lattice.

which is the correct version of (1) in [2]. Note that (3) is the union of pairwise disjoint sets† which will be essential in what follows.

The single point 0, however, does not matter in the calculation of the probabilities wherefore we get

$$1 = \sum_{\ell=1}^{\infty} P(x \in \ell \cdot F_\Lambda) = p \cdot \sum_{\ell=1}^{\infty} \frac{1}{\ell^n} \, . \tag{4}$$

We can thus write p by means of Riemann's ζ-function as

$$p = \frac{1}{\zeta(n)} = \prod_{p \in \mathcal{P}} \left(1 - \frac{1}{p^n} \right) \tag{5}$$

where $\mathcal{P}$ denotes the set of primes [4, 5]. Obviously, $p = 0$ for $n = 1$ (precisely two points are visible here), and p rapidly approaches 1 with increasing n, compare figure 2. For even $n \geqslant 2$, the ζ-function is known to be transcendental [8, 9] (and thus irrational) through $\zeta(2m) = ((2\pi)^{2m}/2(2m)!)|B_{2m}|$, where B_{2m} are the Bernoulli numbers, compare [8]. Also, $\zeta(3)$ is irrational [10], while this question is open for odd $n > 3$. Note that the non-periodicity of F_Λ follows from the irrationality of p, but not vice versa.

A different approach uses the third Möbius inversion formula [3, 4] where one starts from the characteristic function h_Γ of a set Γ, which is one for points of the set and zero otherwise, and rewrites (3) as

$$h_\Lambda = h_{\{0\}} + \sum_{\ell=1}^{\infty} h_{\ell \cdot F_\Lambda}. \tag{6}$$

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† This property would be destroyed by the (unconventional) addition of the origin to the set F_Λ.
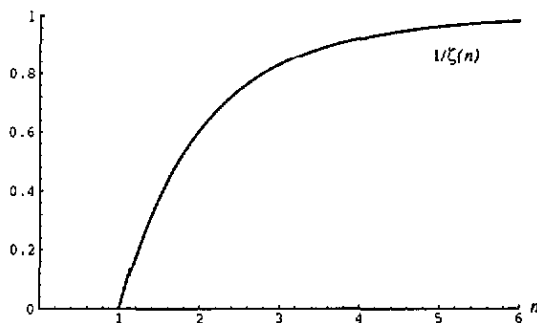
Figure 2. Relative frequency of visible points in a lattice as a function of the dimension.

Convergence is no problem because, for any given point, the right-hand side is a finite sum. Now, using the inversion formula for such series [4] one obtains

$$h_{F_\Lambda} = \sum_{\ell=1}^{\infty} \mu(\ell) h_{\ell \cdot \Lambda \setminus \{0\}} \tag{7}$$

with the Möbius function $\mu(\ell)$, cf. [4]. Note the differences to (1)–(3) in [2] which result from a small mistake in the description of the lattice Λ. It is important though because $|\sum_{\ell=1}^{N} \mu(\ell)|$ does not converge: it is not bounded by $N^{1/2}$ [3, 11].

This indicates that the calculation of the Fourier transform requires some care: it is not clear that the set of visible points is strictly almost periodic in the sense that the Fourier transform need not be a sum over δ-distributions (or Bragg peaks) only. In fact, for $n = 1$, this diffractive part vanishes due to the existence of only two visible points and the Fourier transform is $2\cos(kx)$ and thus continuous. This limit must nevertheless be covered by the correct treatment. In [2], this is hidden by an infinite normalization factor—the formula would give vanishing Fourier transform for $n = 1$.

Let us now consider the so-called structure factor in more detail. The structure factor S_Γ of a discrete set Γ is the Fourier transform of δ-scatterers of equal strength on all points of Γ, i.e.

$$S_\Gamma(k) = \int \sum_{x \in \Gamma} \delta(x' - x) e^{-ikx'} dx' = \sum_{x \in \Gamma} e^{-ikx}. \tag{8}$$

If Γ has inversion symmetry (as Λ and F_Λ do), we can also write $S_\Gamma(k) = \sum_{x \in \Gamma} e^{ikx} = \sum_{x \in \Gamma} \cos(kx)$. Now, with (7), we find

$$S_{F_\Lambda}(k) = \sum_{x \in \Lambda} \sum_{\ell=1}^{\infty} \mu(\ell) h_{\ell \cdot \Lambda \setminus \{0\}}(x) \cdot e^{ikx} \tag{9}$$

to be understood in the distribution sense. Nevertheless, due to lack of convergence, an interchange of the sums is a subtle business. Though a complete treatment is desirable here, it is far beyond the scope of this comment and therefore left to a forthcoming publication [12]. But in the spirit of [2], one can indeed extract the point-like contributions, henceforth called Bragg peaks (though we are talking about *amplitudes* rather than intensities here) because other contributions are arbitrarily small in comparison to the δ-peaks in the thermodynamic limit.

Before we continue, let us remark that the structure factor $S_{F_\Lambda}(k)$ is *periodic* in k WRT the reciprocal lattice Λ^*: we can alternatively write

$$S_{F_\Lambda}(k) = \int \sum_{x \in \Lambda} \delta(x' - x) \cdot h_{F_\Lambda}(x') e^{-ikx'} dx' \tag{10}$$

with the characteristic function h_{F_Λ} defined above. But then, $S_{F_\Lambda}(k)$ is the convolution of $S_\Lambda(k)$—which is periodic !—with the Fourier transform of the characteristic function h_{F_Λ}. Consequently, $S_{F_\Lambda}(k)$ itself is periodic. Furthermore, since the set F_Λ of visible points is invariant under $\mathrm{Aut}(\Lambda)$, the corresponding property applies to its Fourier transform, which is thus invariant under $\mathrm{Aut}(2\pi \Lambda^*)$—the latter again being isomorphic with the group $Gl(n, \mathbb{Z})$. These two arguments apply to the full structure factor (and also to $n = 1$), not only to its Bragg peaks.

To describe the latter, we now consider the reciprocal lattice $2\pi \Lambda^*$ with $\Lambda^* = \{y \mid x \cdot y \in \mathbb{Z} \ \forall x \in \Lambda\} = \mathbb{Z}b_1^* + \cdots + \mathbb{Z}b_n^*, \ b_i^* \cdot b_j = \delta_{ij}$. A Bragg peak sits on every $k = 2\pi(r_1 b_1^* + \cdots + r_n b_n^*)$ with *rational* coefficients, i.e. $r_i \in \mathbb{Q}$. If we write $r_i = p_i/q_i$ with coprime integers p_i, q_i (where we take $q_i > 0$ for convenience), the peaks have strength $H = H(q_1, \ldots, q_n)$,

$$H(q_1, \ldots, q_n) = \sum_{m=1}^{\infty} \frac{\mu(ma)}{(ma)^n} \qquad a = \mathrm{lcm}(q_1, \ldots, q_n) \tag{11}$$

relative to the Bragg peaks of the lattice Λ. Here, lcm denotes the least common multiple. In particular, $q_1 = \cdots = q_n = 1$ gives

$$H(1, \ldots, 1) = \sum_{m=1}^{\infty} \frac{\mu(m)}{m^n} = \frac{1}{\zeta(n)} \tag{12}$$

which is again the frequency of visible points, while H is zero unless *all* arguments are square free, because the Möbius function vanishes for numbers that are divisible by a square. This explains the 'dark' lines in the diagram of intensities (i.e. lines without spots—hence 'white' in figure 3 while really dark in figure 4) which are given—in kinematic approximation—by the absolute squares of the amplitudes (11).

Equation (11) gives a closed formula for the amplitudes of the Bragg peaks in form of an infinite sum, but can still be simplified considerably. If we consider

$$f(n, a) = \sum_{\ell=1}^{\infty} \frac{\mu(\ell a)}{(\ell a)^n} \tag{13}$$

for $\ell, a \in \mathbb{N}$, we can use standard techniques from the treatment of Dirichlet series, compare [5], to evaluate the sum. If $a = p_1 \cdot \ldots \cdot p_r$ is the product of pairwise distinct primes, one can easily show by induction that

$$f(n, p_1 \cdot \ldots \cdot p_r) = \frac{f(n, 1)}{\prod_{j=1}^{r}(1 - p_j^n)} \tag{14}$$

and hence, with the multiplicativity of the Möbius function and (13),

$$f(n, a) = \frac{\mu(a)}{a^n} \cdot \prod_{p \nmid a, \, p \in \mathcal{P}} \left(1 - \frac{1}{p^n}\right) = \frac{1}{\zeta(n)} \cdot \frac{\mu(a)}{\prod_{p \mid a, \, p \in \mathcal{P}} (p^n - 1)} \cdot \tag{15}$$

Inserting this into (11) finally gives, with $a = \mathrm{lcm}(q_1, \ldots, q_n)$, the amplitude function

$$H(q_1, \ldots, q_n) = H(1, \ldots, 1) \cdot \frac{\mu(a)}{\prod_{p \mid a, \, p \in \mathcal{P}} (p^n - 1)} \cdot \tag{16}$$
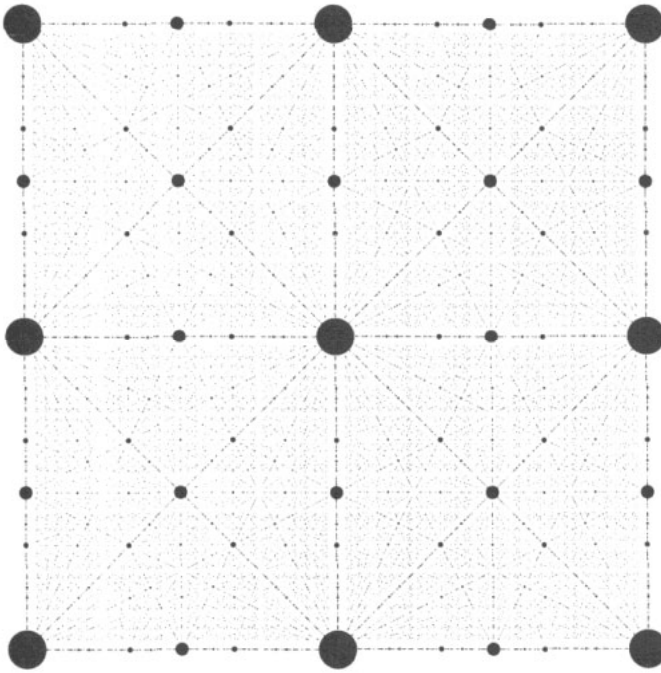
Figure 3. Bragg part of the Fourier transform for the case of the square lattice according to (16). Here, the radius of the dots representing the Bragg peaks are proportional to the amplitude.
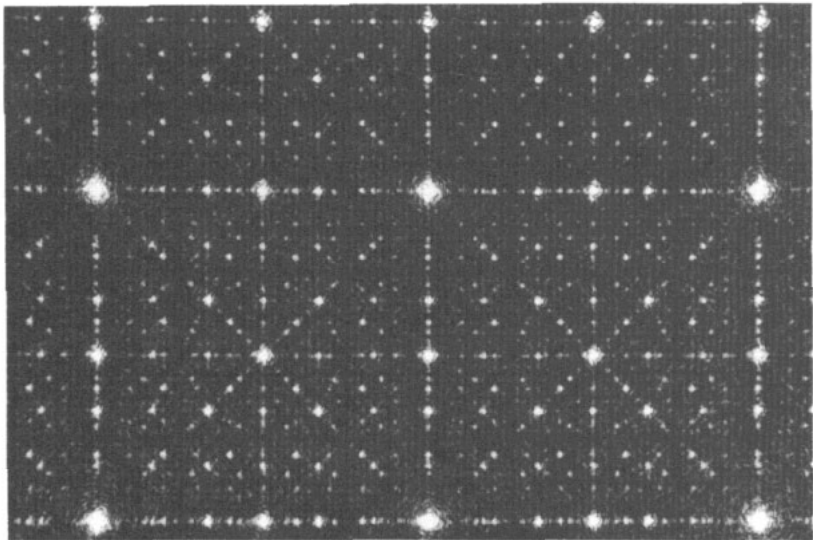

Figure 4. Optical Fourier transform of some 9000 visible points of the square lattice $\mathbb{Z}^2$, see text for details.

This way, the calculation of the amplitudes *relative* to the central amplitude is reduced to the evaluation of a finite product, compare figure 3 for the 2D example of the square lattice. There, a Bragg peak is represented by a dot with radius proportional to the amplitude (i.e.

the area is proportional to the intensity).

The Fourier transform is periodic, although the set itself obviously is not—it is not even quasiperiodic because the Fourier module (i.e. the $\mathbb{Z}$-module generated by the positions of the δ-peaks) is only countably but not finitely generated. The key structure is thus contained in one fundamental domain of the reciprocal lattice. This is indeed clearly seen in figures 3 and 4. The latter was obtained by optical Fourier transform of a finite portion of $F_{\mathbb{Z}^2}$ on an optical bench. Here, we used some 9000 points of radius 15% of the lattice constant. They were prepared as a negative slide made from 24×36 mm^2 documentary film. The light was extracted from a laser beam, widened by a high quality lens to a parallel beam covering the entire slide. Although the image is not perfect (one should not expect rapid convergence in view of the remarks after (9)) and still shows some standard optical errors, it is nevertheless amazing how clear the structure with the subtle invariance properties is recovered. It is correctly described by the approach via the Möbius transform while previous numerical attempts [1] seem to fail for reasons we were not able to unravel.

Of course, one can now deal with generalizations like the set of points visible to two or more observers which resembles the above situation in many respects, although the relative position of the observers does play a significant role. Unfortunately, we could not find similarly nice closed expressions for the Fourier transform wherefore we drop further details here.

Acknowledgments

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